OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

INFORMATICS MATTERS
SOLUTIONS FOR DRUG DISCOVERY

OpenRiskNet: an open e-infrastructure to support data sharing, knowledge integration and *in silico* analysis and modelling in risk assessment

Tim Dudgeon (IM), Thomas Exner (DC), Joh Dokler (DC), Daniel Bachler (DC), Lucian Farcal (DC), Chris Evelo (UM), Egon Willighagen (UM), Marc Jacobs (Fraunhofer), Philip Doganis (NTUA), Haralambos Sarimveis (NTUA), Iseult Lynch (UoB), Stefan Kramer (JGU), Cedric Notredame (CRG), Danyel Jennen (UM), Georgios Gkoutos (UoB), Ola Spjuth (UU), Paul Jennings (VU), Frederic Bois (INERIS) and Barry Hardy (DC)

Tim Dudgeon | tdudgeon@informaticsmatters.com
www.openrisknet.org

Introduction

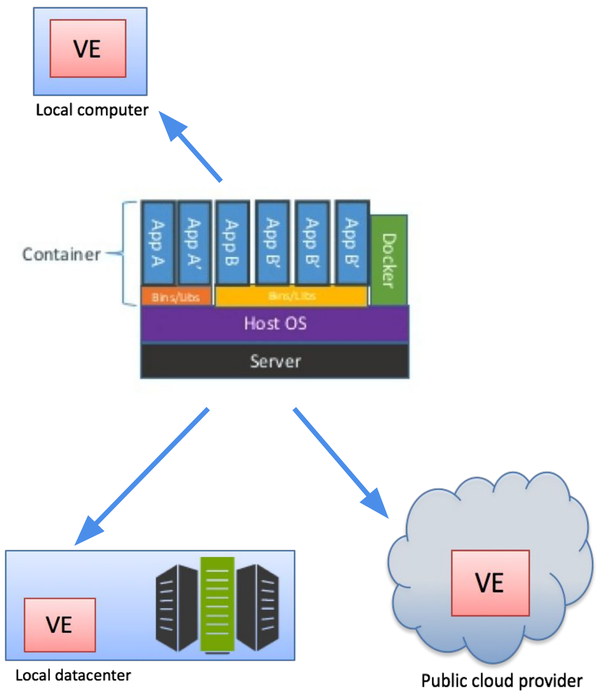
OpenRiskNet is

- a virtual research environment for **predictive toxicology** and chemical and nanomaterial **risk assessment,**
- **harmonising** access to data and facilitating **interoperability** of software,
- easily **deployable** to single computers, public and in-house cloud solutions,
- addressing the needs of **industry and academic researchers, risk assessors, regulators and informed public.**

Service-oriented science, containerization, deployment

- Uses modern and established tools and frameworks supported by industry
- Offers an agile and scalable environment to use, and a straightforward platform to extend

- Allows language-agnostic integration of diverse software
- Reduces extra work for integration
- Reduces risk and improve sustainability



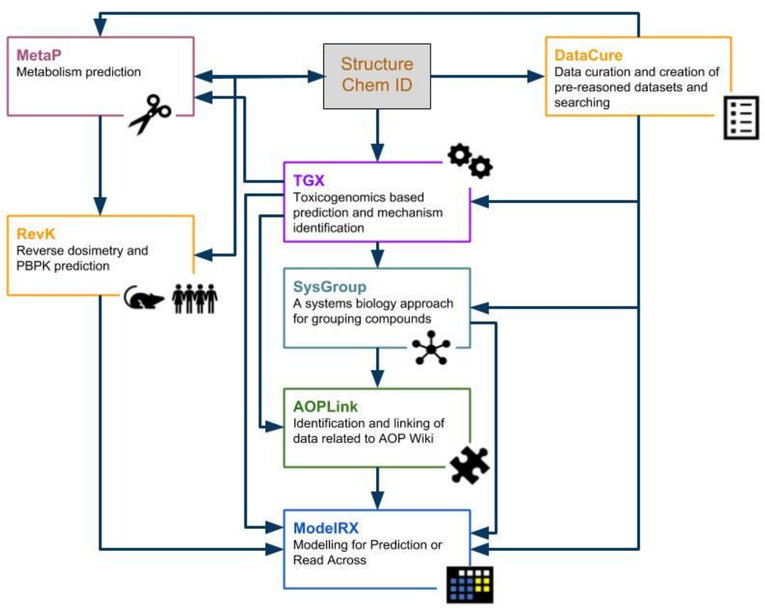
Main concepts:

1. **REST services** providing data and processing/analysis/modelling tools (provided by OpenRiskNet and associated partners)
2. **Harmonize APIs** in an bottom-up approach
3. Microservice architecture based on **containerization and container orchestration** accompanied by a **discovery service**
4. **Virtual infrastructures**, which can be deployed on public or in-house clouds - reference environment available at https://home.prod.openrisknet.org

Case studies

Case-study-driven development is used to
- test and evaluate the solutions provided,
- demonstrate the ability to satisfy stakeholder groups requirements,
- present real-world applications,
- guide the prioritization of data sources and tools.

A workflow for the safety assessment of chemicals without animal testing developed within the **SEURAT-1 project** (Berggren et al., 2017) was selected to guide the definition of 7 case studies. This workflow constructs a hypothesis based on existing data, computational modelling, biokinetic considerations, and then, targeted non-animal testing.



Associated partner program

This Programme aims at strengthening the working ties between the OpenRiskNet Consortium members and other organisations within relevant scientific and technology communities. Any organisation such as a university, institute, consortium, non-governmental organisations (NGOs), as well as SMEs and large commercial companies can become an Associate Partner.

We expect to have these types of users:
1) **service providers**, which would like to integrate their databases and software tools into the OpenRiskNet infrastructure.
2) **early adopters**, who will use the infrastructure for their predictive toxicology and risk assessment tasks.
3) **technology partners**, which develop services and tools on which the OpenRiskNet e-infrastructure will be based.

To be able to share all information and include you directly in the design process of OpenRiskNet, we would like to ask you to sign a short legal agreement with us. Additional information on how to become an Associated Partner to OpenRiskNet is available at:
https://openrisknet.org/docs/Associated_Partner_Programme_Agreement-Guidelines.pdf

Implementation challenge

The Implementation Challenge has been created to select external tools that can be integrated into the OpenRiskNet infrastructure. The scientific advisory board will work together with the coordinator and the WP leaders to prioritize the proposed services and select the winning groups.
Funding and the technical support can be provided to cover the work associated with making the service OpenRiskNet compliant. This includes the adoption of the OpenRiskNet API concept including the interoperability layer, generation of the data schemata for in- and output as well as containerization and deployment.
€6.000 - €12.000 (in-kind work contributions) can be provided depending on the complexity of the service to be integrated and the amount of adaptations needed.

Deadlines for applications for the implementation challenges are:
- 30 September 2018
- 31 December 2018
- 30 April 2019

Winners will be announced shortly after each deadline.
More information is available at:
https://openrisknet.org/associated-partner-programme/implementation-challenge

OpenRiskNet partners

P1 Douglas Connect GmbH, Switzerland (DC)
P2 Johannes Gutenberg-Universität Mainz, Germany (JGU)
P3 Fundacio Centre de Regulacio Genomica, Spain (CRG)
P4 Universiteit Maastricht, Netherlands (UM)
P5 The University Of Birmingham, United Kingdom (UoB)
P6 National Technical University Of Athens, Greece (NTUA)
P7 Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., Germany (Fraunhofer)
P8 Uppsala Universitet, Sweden (UU)
P9 Medizinische Universität Innsbruck, Austria (MUI)
P10 Informatics Matters Limited, United Kingdom (IM)
P11 Institut National de l'Environnement et des Risques INERIS, France (INERIS)
P12 Vrije Universiteit Amsterdam, Netherlands (VU)

References and more information

Elisabet Berggren, Andrew White, Gladys Ouedraogo, Alicia Paini, Andrea-Nicole Richarz, Frederic Y. Bois, Thomas Exner, Sofia Leite, Leo A. van Grunsven, Andrew Worth, Catherine Mahony, "Ab initio chemical safety assessment: A workflow based on exposure considerations and non-animal methods", Computational Toxicology, Volume 4, 2017, Pages 31-44.

https://openrisknet.org/development/api-concept/
https://openrisknet.org/development/case-studies/
https://json-ld.org/spec/latest/json-ld/
https://www.openshift.com/

Acknowledgements

OpenRiskNet (Grant Agreement 731075) is a project funded by the European Commission within the Horizon2020 Programme